Imperial College London

Software Sustainability Institute

Hi, I'm Lucy! And I'm a.....

...materials scientist = *physics + chemistry + engineering*

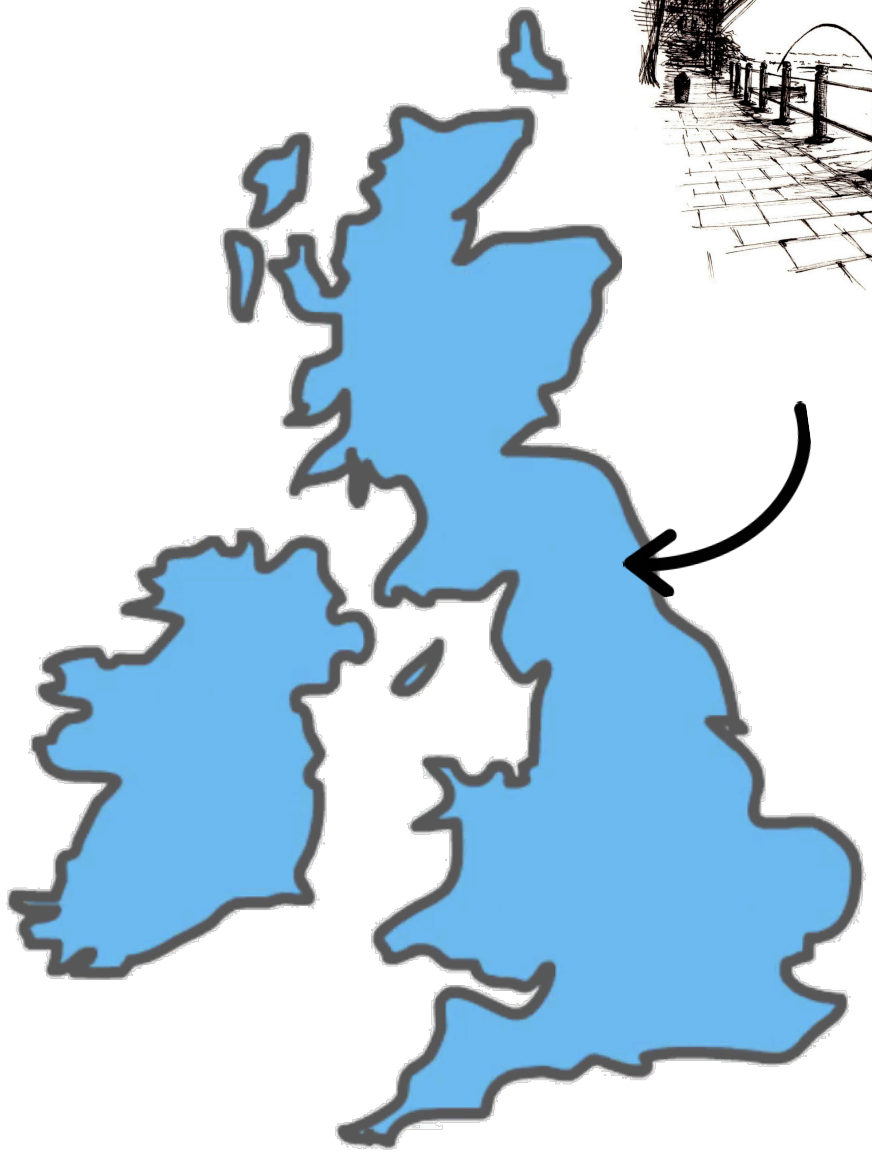
Stephanie Kwolek

Kevlar

Bullet-proof vest

...woman

About Me

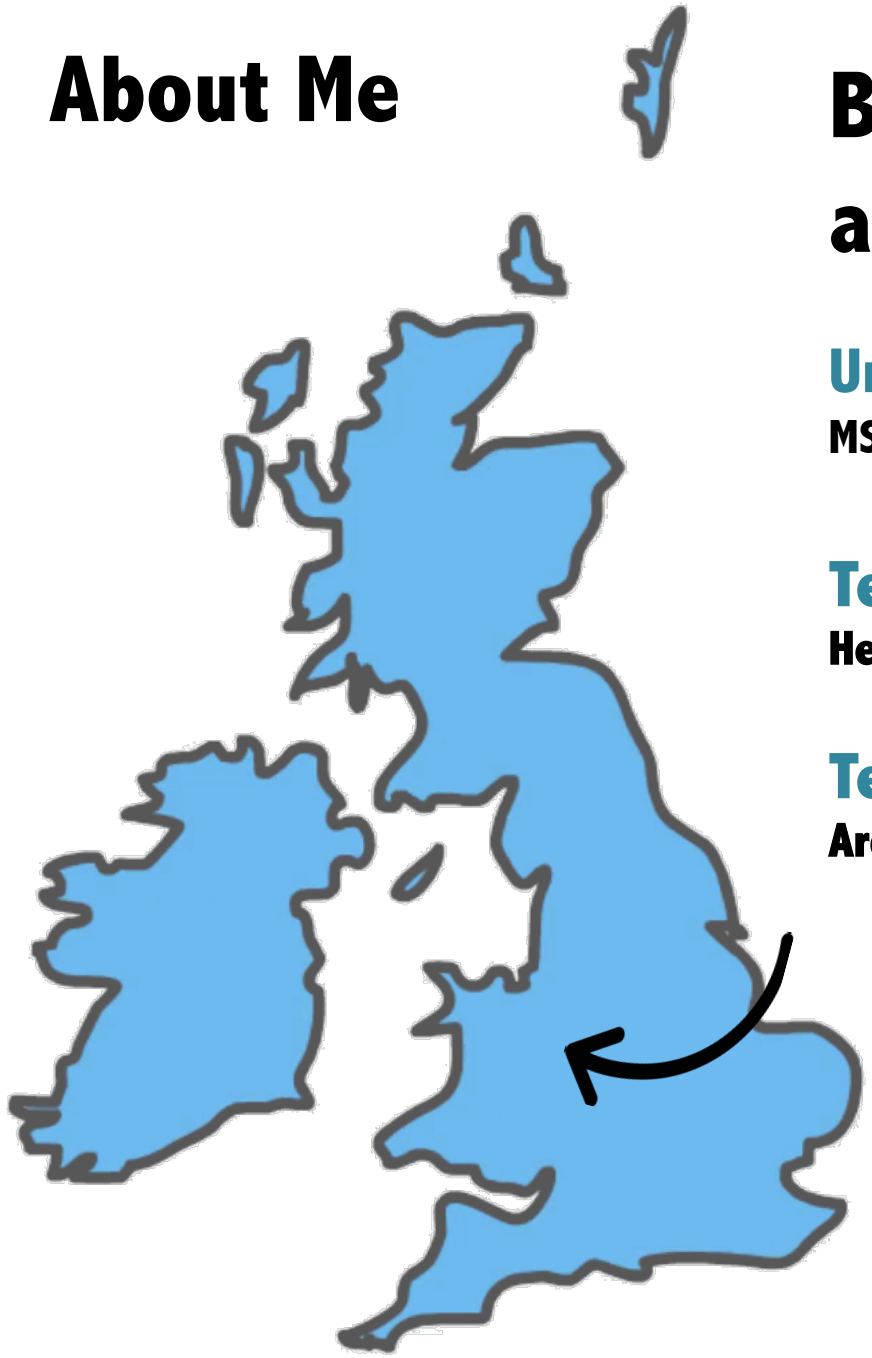


Newcastle (19 years)

A-levels

Maths, Further Maths, Physics, Philosophy

About Me



Birmingham: university and teaching (12 years)

Undergraduate degree

MSci Theoretical Physics

Teaching qualification

Her Majesty's Prison Birmingham

Teaching job

Arden Primary School

About Me

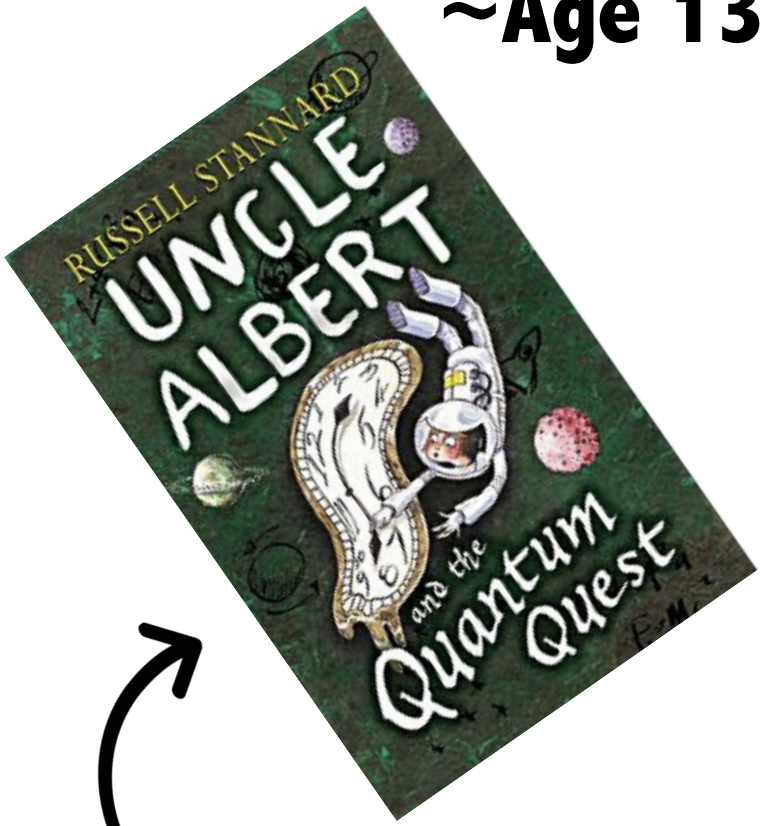
London: PhD work (4 years)

PhD student

Materials Science

Why did I choose physics?

~Age 13

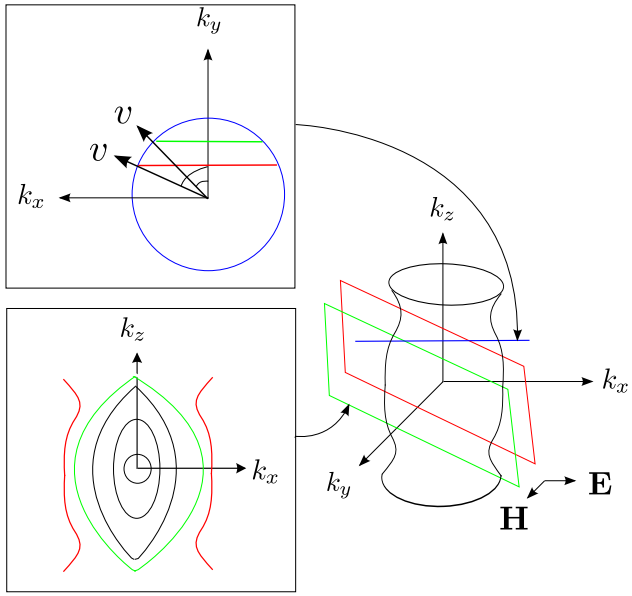


Quantum Mechanics

~Age 16

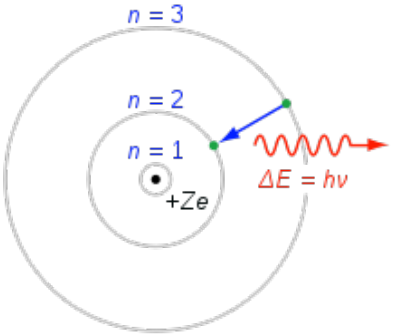
Computing / Programming

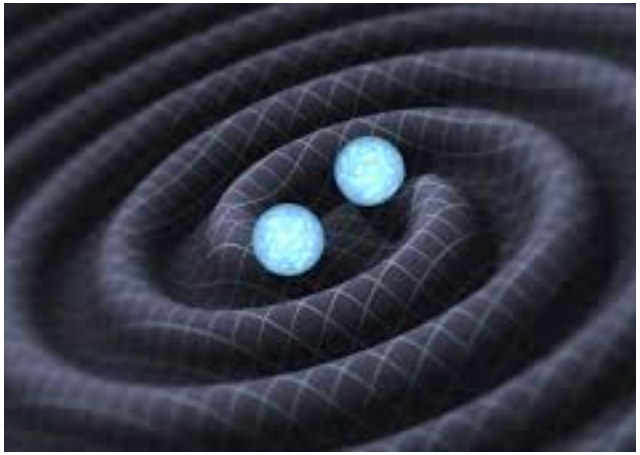
MSci Theoretical Physics



research project: modelling electrons in a quasi-2D metal

Lots of quantum mechanics (lots of maths)





summer project: analysing gravitational wave data

Why did I leave physics?

1. I couldn't find a physics question that I cared about enough

2. I didn't think I was good enough…

Why did I leave physics?

Why did I return?

1. I couldn't find a physics question that I cared about enough

   I found out about materials science (energy materials)

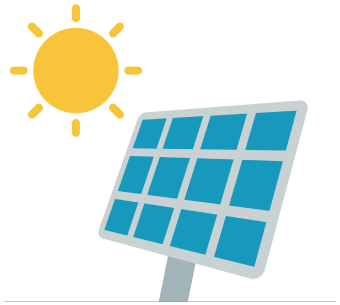
2. I didn't think I was good enough…

   I decided to ignore that voice in my head

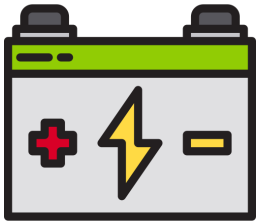
Energy materials

= materials that generate and store energy

solar cells



batteries

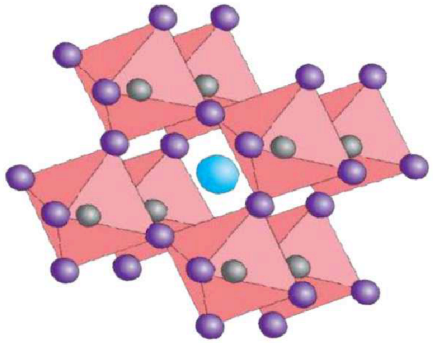


To replace fossil fuels we need new cheap, long-lasting materials made from abundant elements

To design new materials we need physics!


ON BEHALF OF LIFE
CLIMATE CHANGE:
12 YEARS TO SAVE EARTH

Computational modelling



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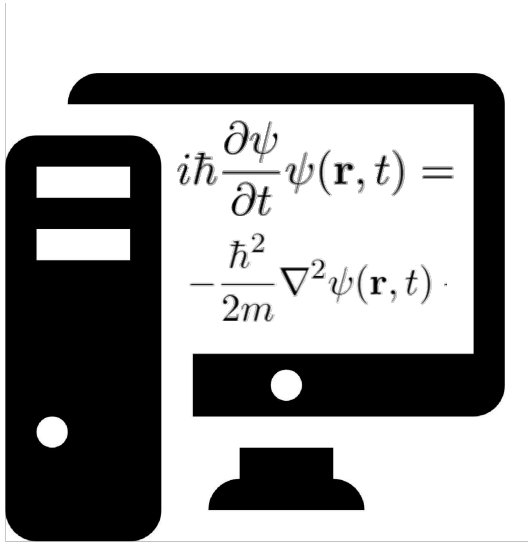


- *mechanical*
- *electrical*
- *thermal*
- *optical*
- *magnetic*

Input:
atomic structure

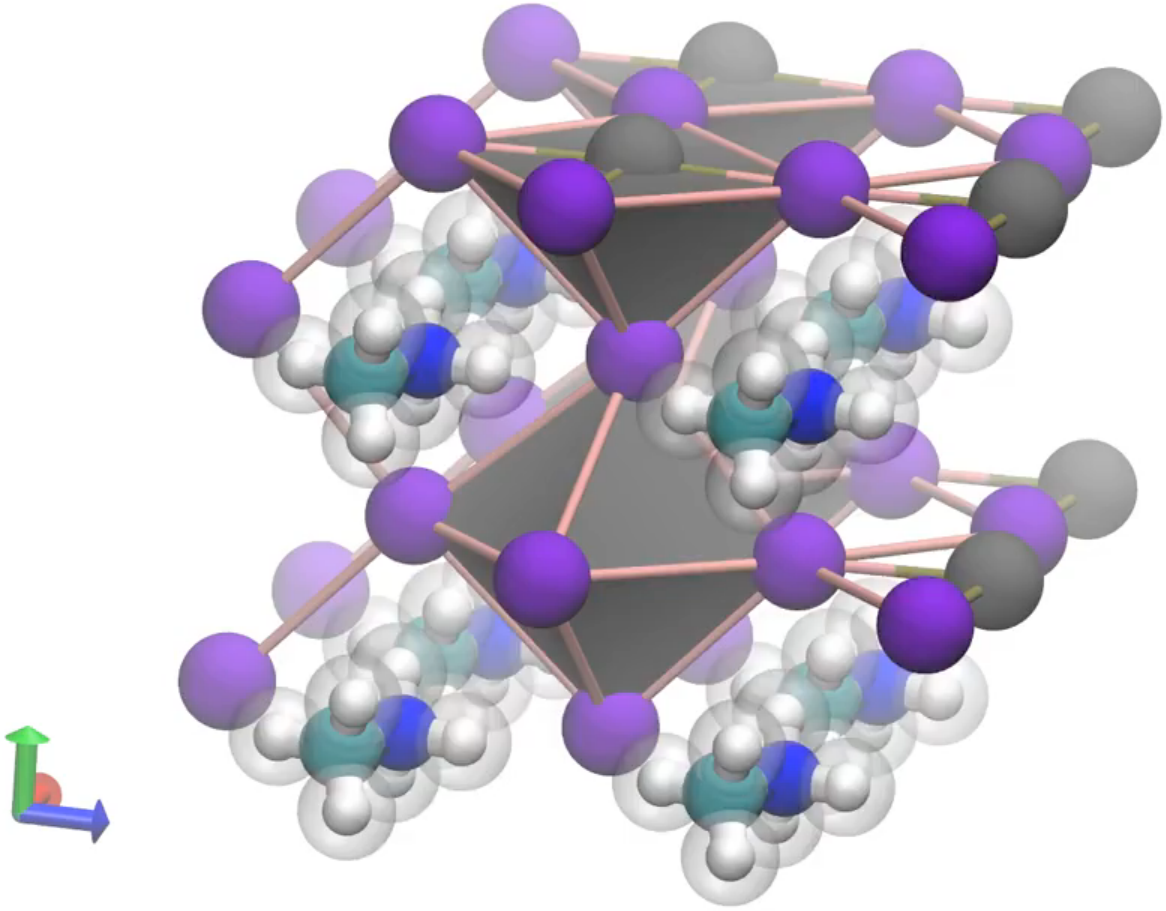
Solve QM equations

Output:
material properties

Computational modelling can be used to develop new materials

Example: vibrations in a solar cell material

(video courtesy of Jarvist Moore Frost)



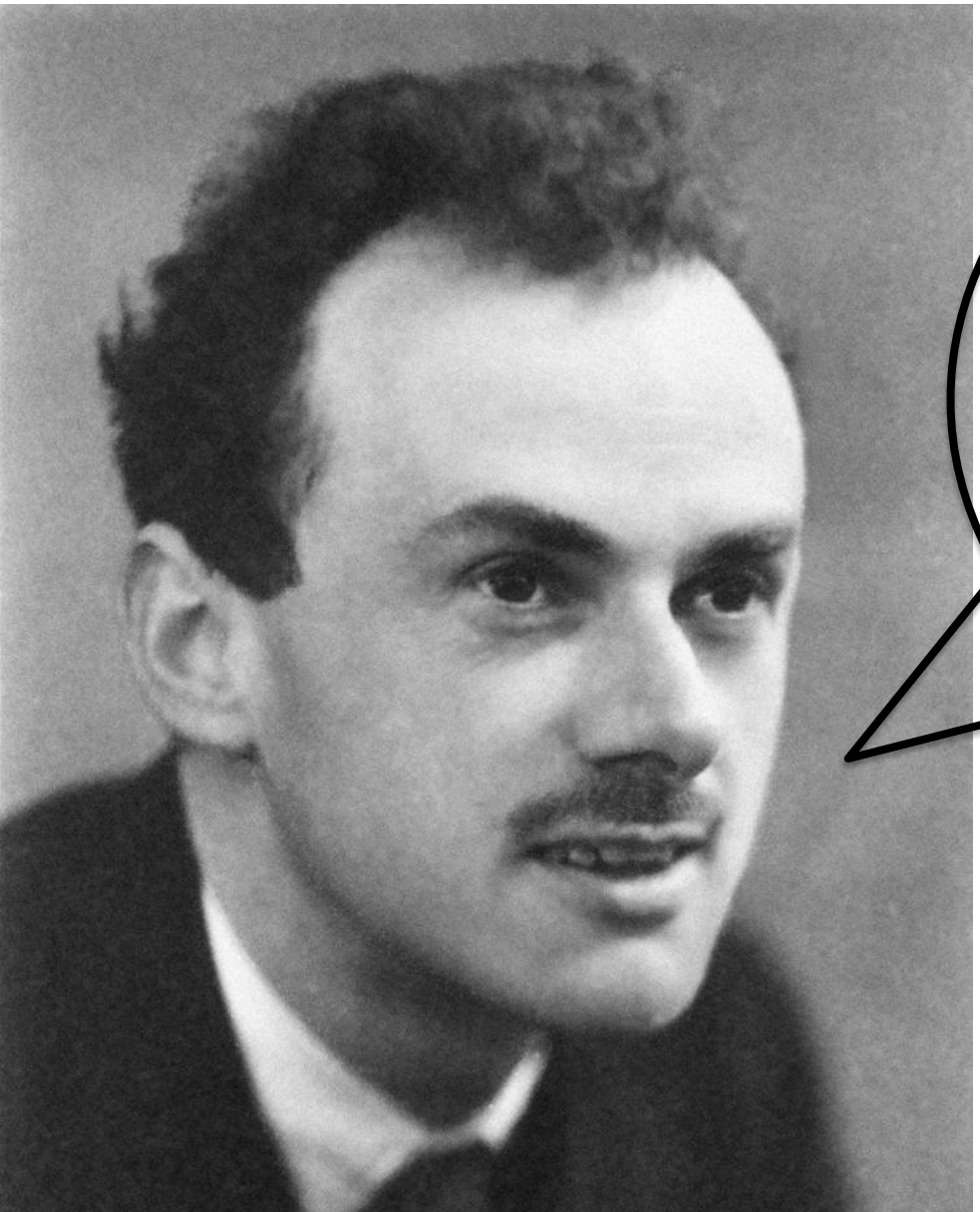
Ab-initio computational modelling

$$i\hbar\frac{\partial\psi}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t)$$

The Schrodinger Equation

1926

Ab-initio Computational modelling

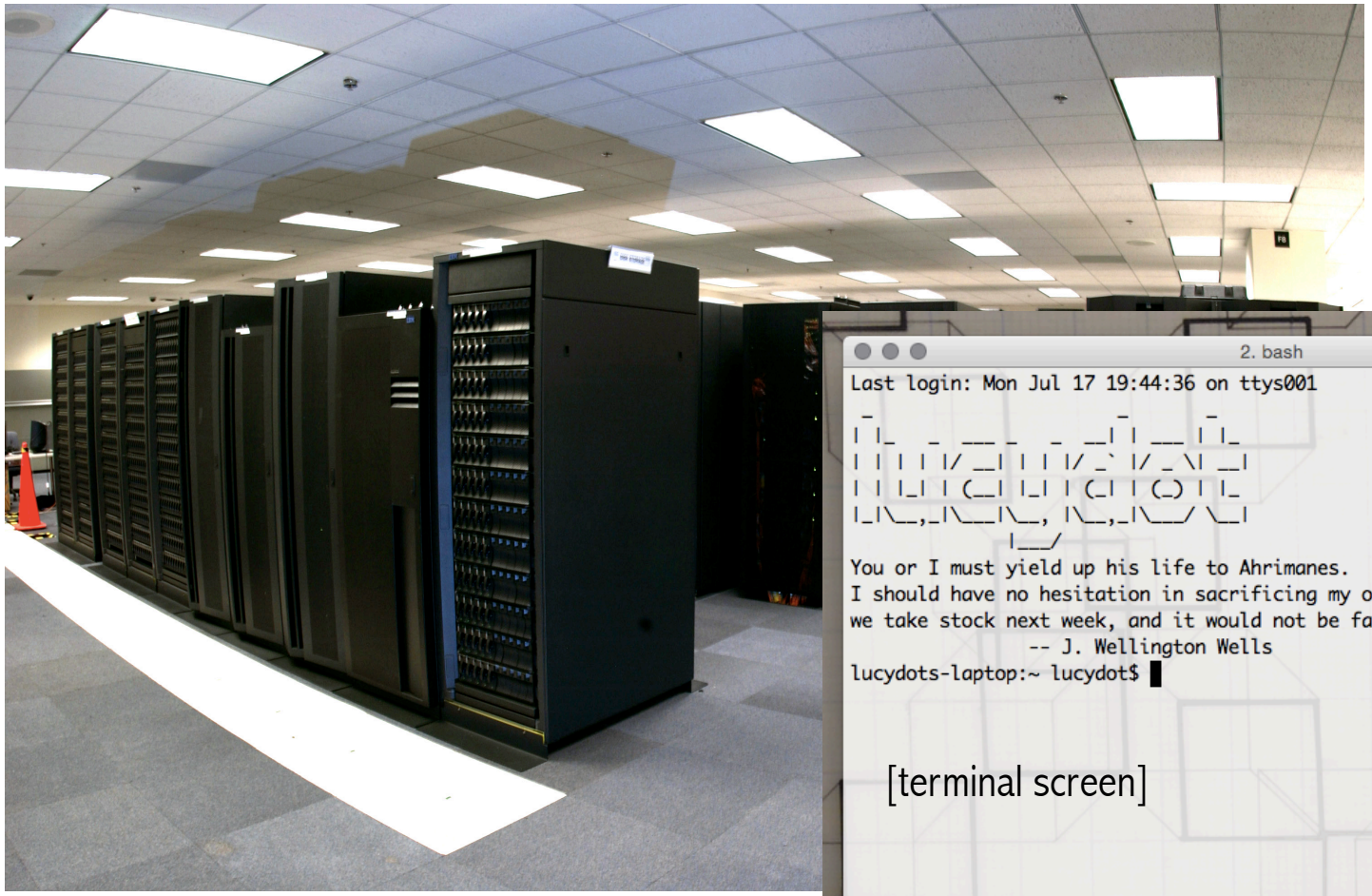


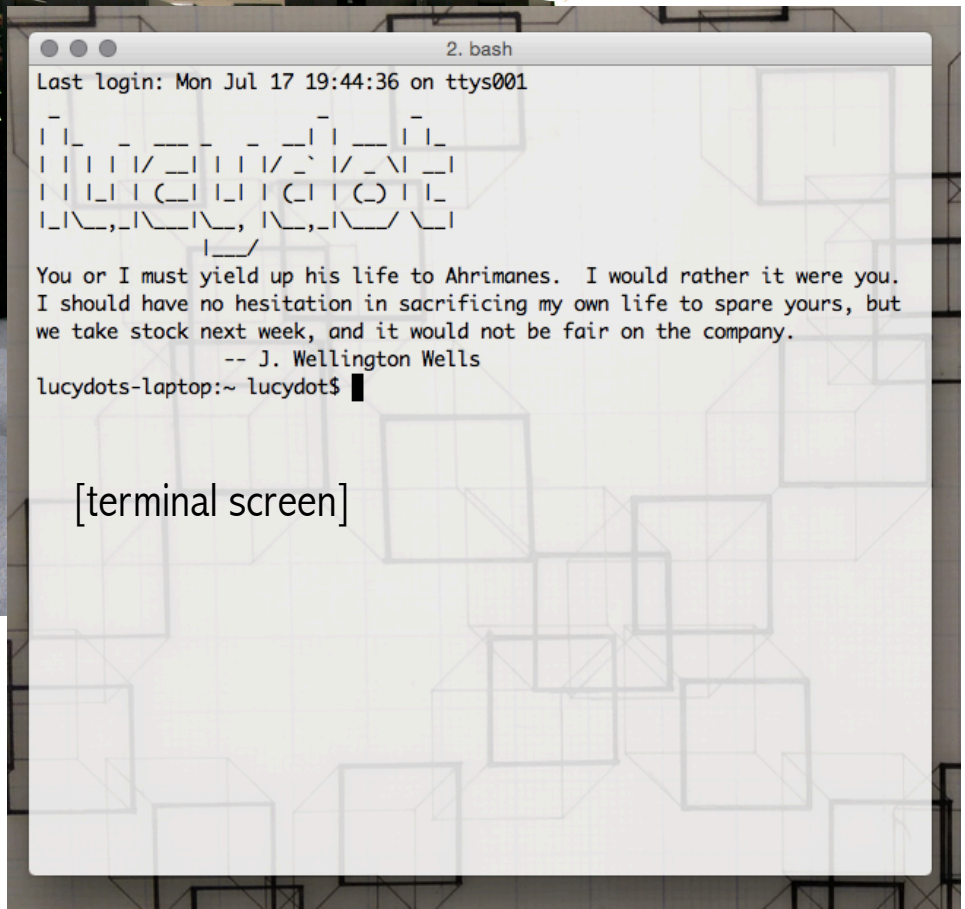
"The underlying physical laws necessary for a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact applications of these laws lead to **equations much too complicated to be soluble.**"

Paul Dirac

1929

This is my lab…supercomputers!



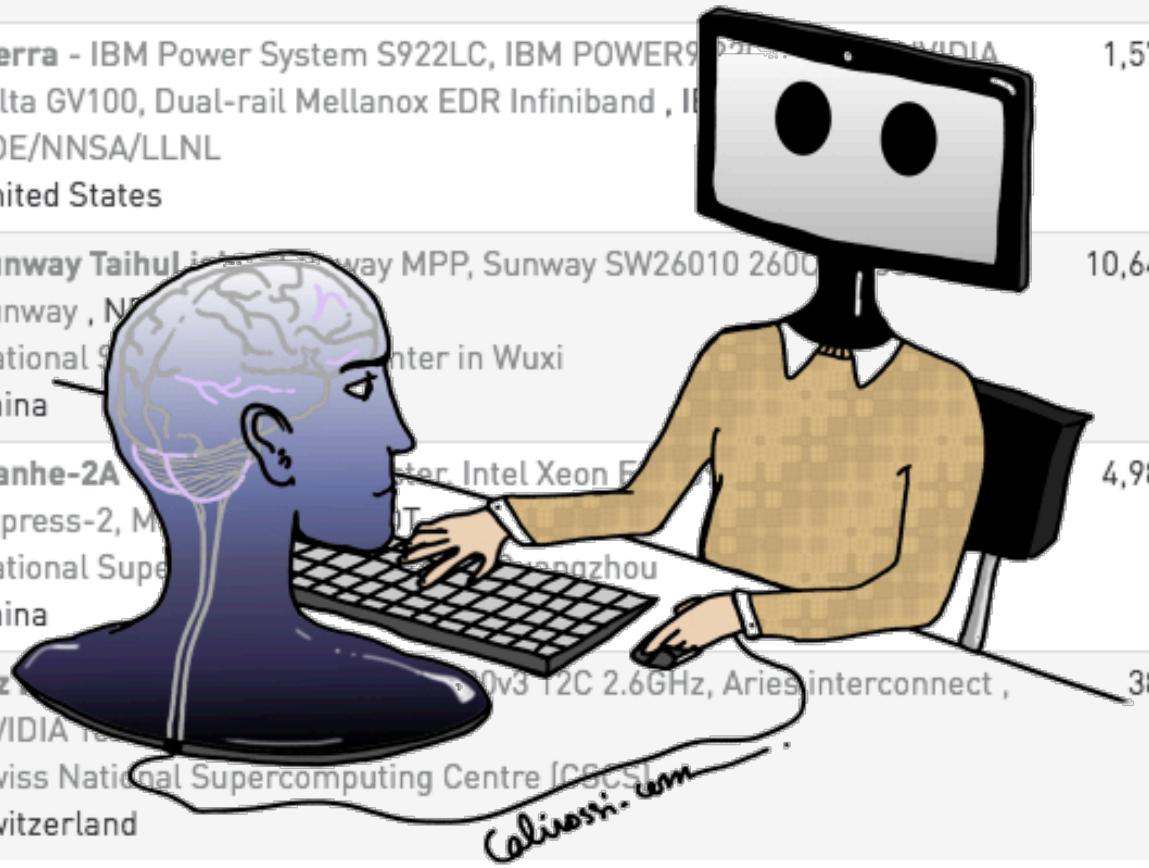


[terminal screen]

Fastest supercomputers in the world

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,397,824	143,500.0	200,794.9	9,783
2	**Sierra** - IBM Power System S922LC, IBM POWER9 [illegible] NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , I[illegible] DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
3	**Sunway Taihul[illegible]** way MPP, Sunway SW26010 260[illegible] Sunway , N[illegible] National S[illegible]nter in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
4	**Tianhe-2A** [illegible]ter, Intel Xeon E[illegible] Express-2, M[illegible]OT[illegible] National Supe[illegible]uangzhou China	4,981,760	61,444.5	100,678.7	18,482
5	**Piz[illegible]** [illegible]0v3 12C 2.6GHz, Aries interconnect , NVIDIA [illegible] Swiss National Supercomputing Centre (CSCS) Switzerland	387,872	21,230.0	27,154.3	2,384

> 1 exaflop/s
(> 1000000000000000000 flops/s)



The problem with Einstein

Don’t just think about academic labels (history, physics, business) ***– think about the type of question you want to answer***

It is easy to doubt your ability ***– it’s normal to feel unconfident when you’re doing difficult work***
– GO FOR IT

Thank-you! 

Slides : lucydot.github.io/slides